UCRL-MI-125919

Application and Implementation of the ParFlow Groundwater Flow Model

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This paper was prepared for submittal to the
Advanced Simulation of Subsurface Flow and Containment Transport Conference
Research Triangle Park, NC
December 5-6, 1996

January 1997

Lawrence Livermore National Laboratory

UCRL-JC-125919 Ext Abs

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The ParFlow model is being designed and developed to rapidly simulate saturated groundwater flow and chemical migration processes in large-scale, three-dimensional geologic formations. By "large-scale", we refer to application problems that are both large in their spatial extent and detailed with respect to spatial resolution. These conditions are often generated by the need to understand the impacts of small-scale geologic heterogeneity (on the order of 1 to 10 m) on the rates of groundwater flow and patterns of tracer or chemical migration that evolve over much larger scales (say between 100 to 1000 m, or more). The relevant computational problems can often exceed millions or tens of millions of unknowns.

The interest and detail in this type of problem has largely been motivated by nationwide efforts to assess and remedy groundwater quality problems associated with industrial or defense complex contamination, long term agricultural practices, and broader groundwater resource management issues. In this context, groundwater simulations are typically used to provide a rational basis for analyzing issues related to long-term health risks, natural attenuation behavior, the cost-effectiveness of contamination remediation technologies, and so forth.

Historically, oversimplified conceptualizations of system behavior have been used as the basis for many types of design and modeling studies. The role of geologic heterogeneity has not been frequently considered, even though its impact in many instances is becoming increasingly apparent and relevant. Although simplified approaches are usually justified in some sense by the lack of sufficient characteristic geologic data (to fully specify the distribution of heterogeneous properties, for example), they do nothing to scientifically address or quantify the uncertainties implied by the paucity and variability of information usually available. This can lead to unreliable and over-engineered remedial solutions that are unnecessarily expensive. Practical techniques for dealing with the important effects of heterogeneity in geologic systems are few and far between.

Our approach for "dealing" with heterogeneity involves the use of ParFlow to enable large-scale, highly-resolved simulations of flow, transport and reaction phenomena in systems that recreate the character and detail of physical and chemical variability observed in natural physical formations. This is achieved through the use of multiple, equally likely stochastic "realizations" of the system heterogeneity within known, or deterministic, structural boundaries of a formation. It is meant to complement and bridge the gap between theoretical (e.g., stochastic) models and various laboratory and field experimental studies focused on discerning the important features and impacts of heterogeneity.

ParFlow has been developed for use on a variety of computational platforms, ranging from large-scale, massively parallel computers such as the Cray T3D, to smaller clusters of engineering workstations, to Windows 95 PC's. It has been optimized for repeated large-scale flow simulations by incorporating a concise, hierarchical, and grid-independent representation of hydrostratigraphic flow units, direct generation of the stochastic property fields via several parallel generation techniques, and an efficient solution of the discretized equations using a multigrid preconditioned conjugate gradient (MGCG) technique.

The use of repeated "Monte Carlo" simulations allows the uncertainty associated with any one stochastic simulation to be quantitatively bracketed by the results of the ensemble. Nevertheless, it reinforces the need to achieve efficiency in any one simulation so that all may be accommodated. To this end, the MGCG technique was developed as the core of the ParFlow flow model. MGCG combines the scalability and speed of multigrid algorithms (i.e., the convergence rate is preserved regardless of problem size) with the guaranteed convergence properties of conjugate gradient methods.

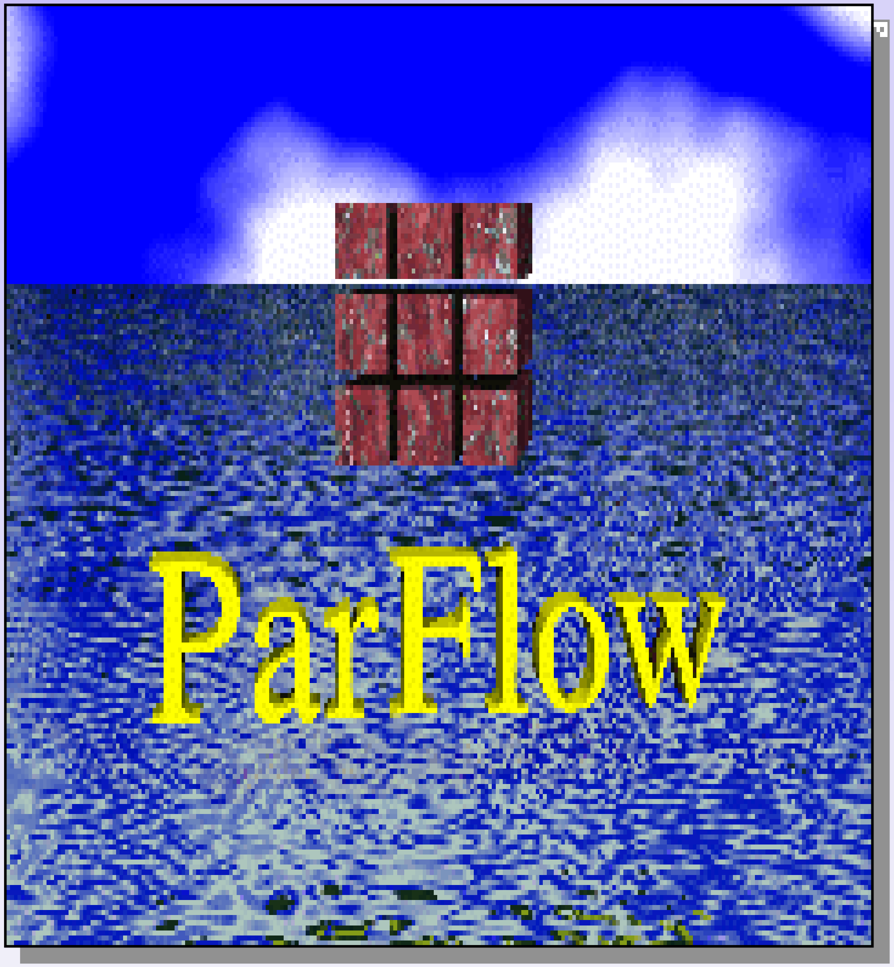
The entire process of doing multiple realization simulations implies that additional efficiencies with respect to data manipulation be developed. This point is made clear by the fact that importing and exporting millions of property and simulation data values can dominate the wall-clock time of any one simulation. With this in mind, domain, geostatistical, boundary condition, and other conceptual model specifications for a given problem occur in ParFlow through a series of grid-independent inputs. These serve to reduce the volume of input data required for one or more Monte Carlo runs. At run time, a grid resolution is specified, and the requisite interpolation and property assignments onto the grid are done automatically. Moreover, internal routines for the parallel generation of stochastic property fields (currently including a parallel Turning Bands method and a conditional Parallel Gaussian algorithm) are also invoked. In addition, newer features for real-time graphical output and solution interrogation and assessment are also being developed. Although the grid-independent approach was motivated by the need to minimize I/O choke points in large problems, it also allows the early stages of conceptual model development to be unencumbered by concerns related to the grid and its optimal size. Because of ParFlow's portability, much of the time-consuming initial aspects of conceptual model development and testing can now be relegated to smaller computers.

At this time, the transport component of the ParFlow model includes an explicit Godunov advection routine for the simulation of non-dispersive transport of dilute (neutrally buoyant) solutes within the steady groundwater flow regime. This capability is currently complemented by an external serial particle-grid transport model (SLIM). Although the Godunov scheme also forms a basis for multiphase flow components of Parflow now under development, its transport performance is hampered by extreme time-step limitations produced by locally large velocities near wells or in fast flow channels in the formation. These issues will be ameliorated to some extent by the incorporation of temporal sub-cycling technique to localize the small time step calculations in areas where they are required, and also by the inclusion of an internal particle transport model within ParFlow.

During the presentation, several example applications of ParFlow will be shown. These will serve to illustrate ParFlow's computational performance on several test problems and document its application to several field and contaminant remediation sites in California. Additional modifications to ParFlow to improve its practical applicability and future potential applications of this modeling approach will also be discussed.

This work was performed under the auspices of the U.S. Dept. of Energy at LLNL under contact no. W-74-5-Eng-48.

Application and Implementation of the ParFlow Groundwater Flow Model



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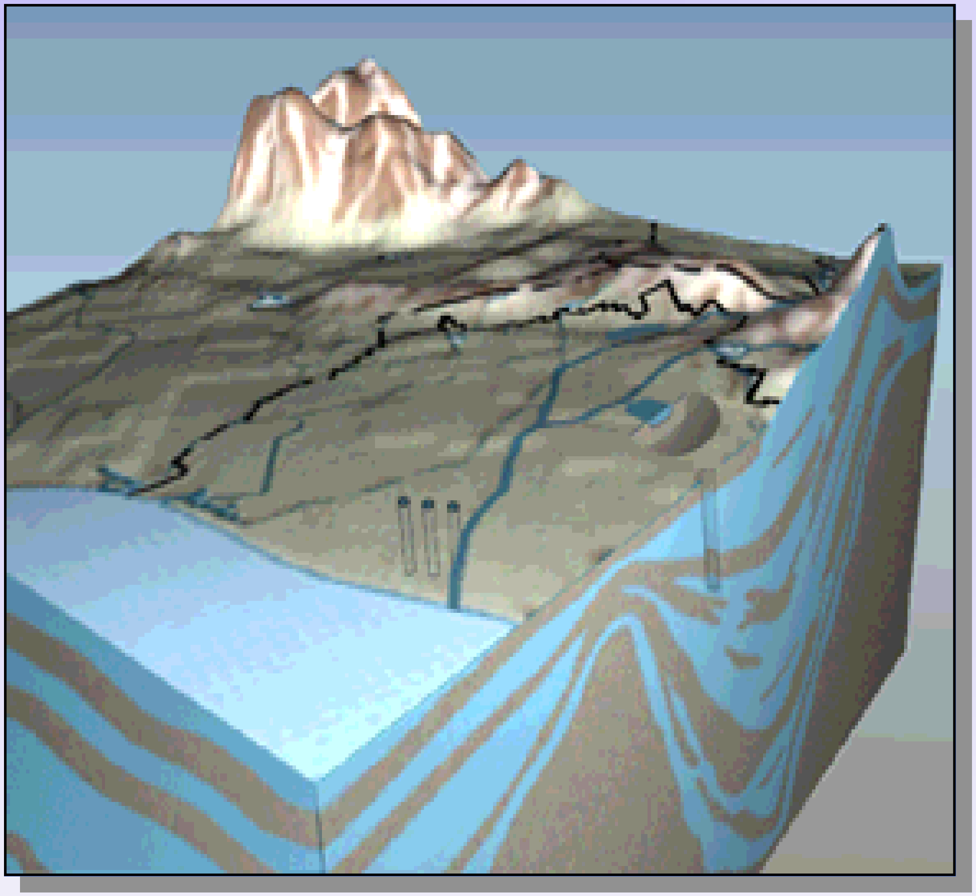
- Motivation and role
- Design and performance aspects
- Survey of recent applications
- Future development issues
- Some video highlights

ParFlow is Designed for Rapid Simulation of Flow and Transport in Large, Heterogeneous Systems

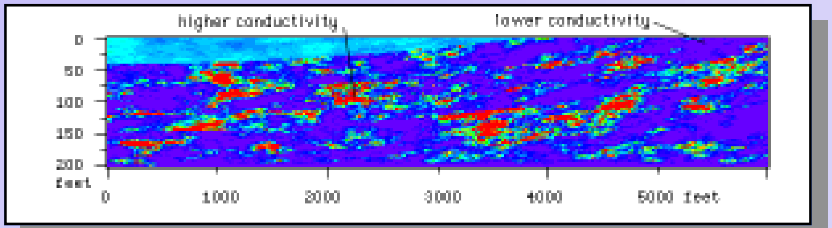


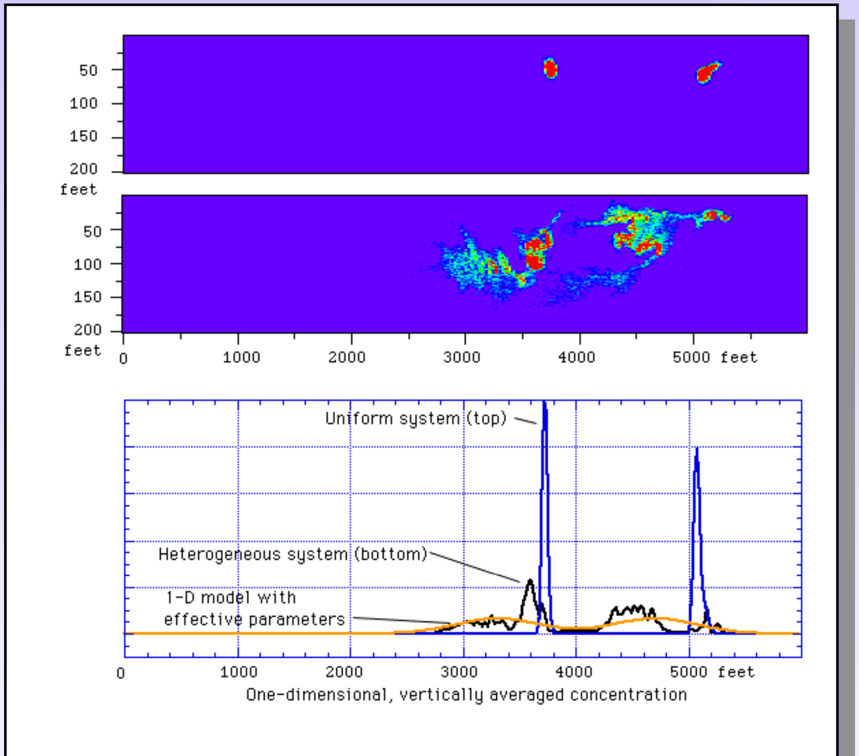
- 3D systems that are large in their spatial extent (km)
- 3D systems that require fine resolution (m) to represent nonuniform properties and important small-scale process interactions
- Rapid simulation allows “Monte Carlo” analyses to bracket risk and other assessments of uncertainty
- For many problems in hydrology and petroleum engineering, “heterogeneity” is the name of the game

Heterogeneity is **Reality** in the Subsurface

- Variable formation materials and properties
- Preferential flow and migration pathways
- Nonuniform soil reactivity
- Impossible to measure medium properties in full detail
- Importance of 3-dimensional behavior
- Uncertain implications for prediction of:
  - chemical or tracer transport
  - contaminant remediation
  - perturbations in aqueous geochemistry

We Deal with Heterogeneity via Direct Simulation





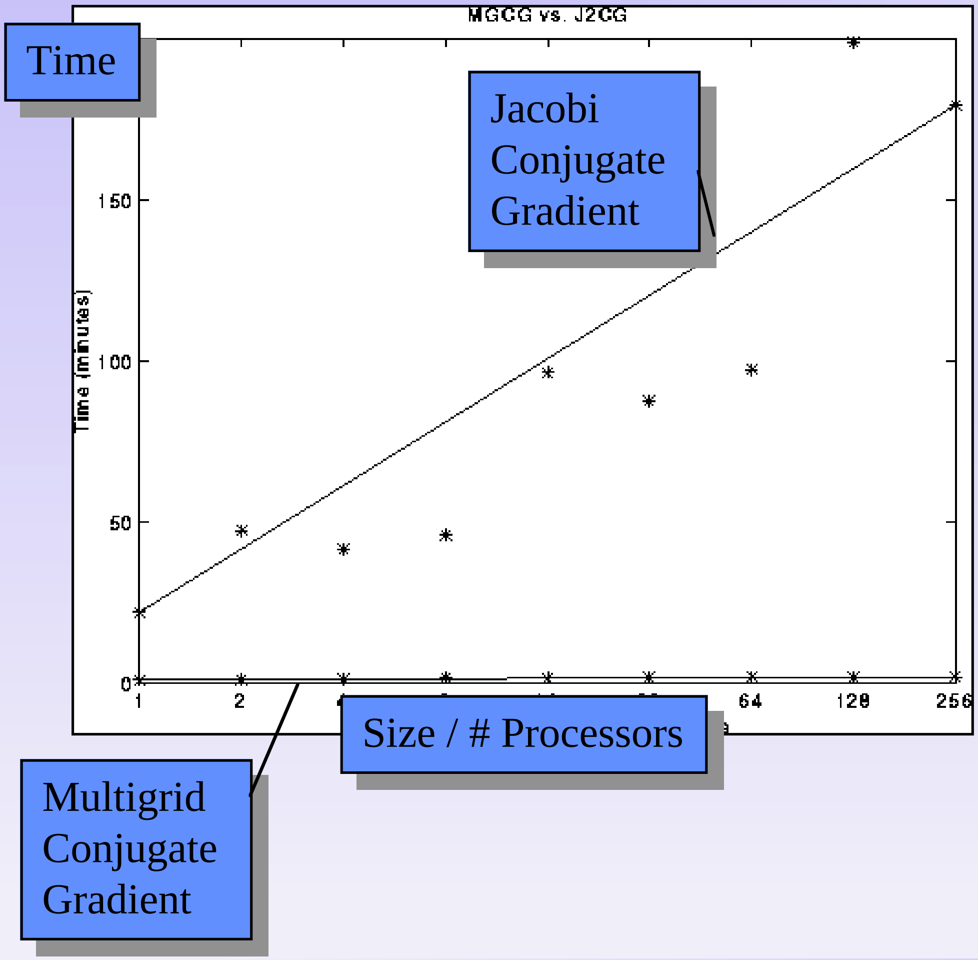
- Geostatistical representations of medium properties
  - use all data as opposed to averaged values
  - incorporate “hard” measurements, “soft” data, qualitative geologic interpretation
  - respect geologic “plumbing”
- Monte Carlo approach allows uncertainty of one run to be bracketed by “ensemble”
- Requires significant computational power
- May be only way to predict complex interactions in complex field systems
- Valuable surrogate for field tests
- Bridge gap between “homogenization” theories and research field sites

Our Approach Relies on Scaleable Algorithms, Efficient Domain Specification, and Platform Portability

- Components of ParFlow
  - Scaleable Multigrid Preconditioned Conjugate Gradient (MGCG) solver
  - nested generation of stochastic property fields
  - grid-independent domain specification
  - explicit 2nd order Godunov advection routines
  - platform portability

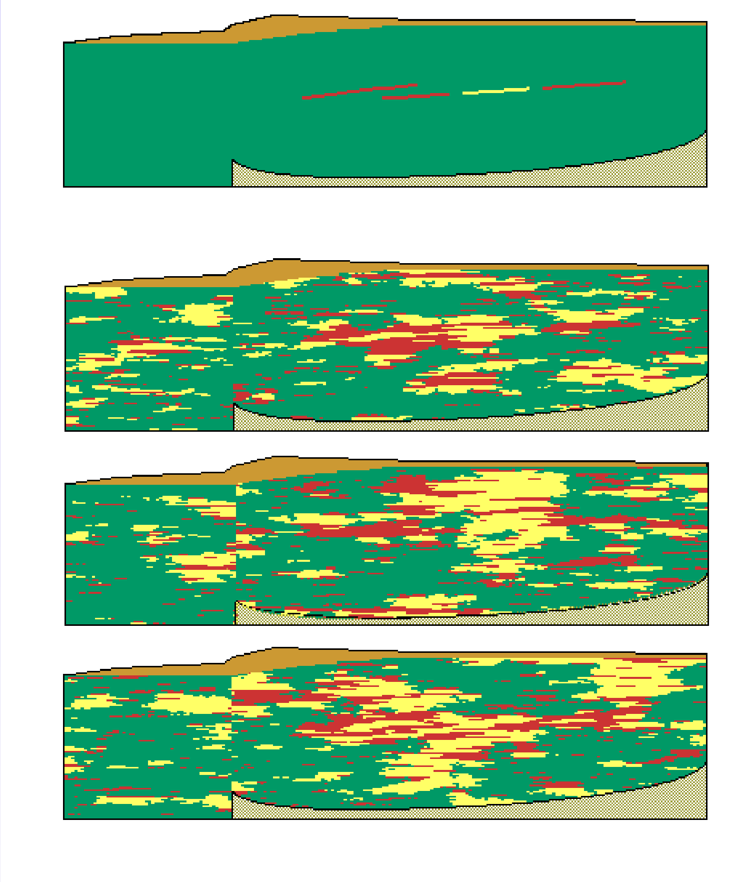
- Monte Carlo efficiency must envelop all model components
- Scaleable algorithms
  - Stable MGCG iteration counts for increasing problem size
- Scaleable parallel implementations
  - Bigger Problems + Additional Processors = Comparable Run Times
- Portability of ParFlow across multiple platforms —
  - parallel machines (T3D), engineering workstations (Sun), Windows 95 PCs
  - flexibility allows conceptual design to occur on smaller machines, larger runs on bigger machines

Multigrid Preconditioned Conjugate Gradient Algorithm Forms the Core of the Steady Flow Module



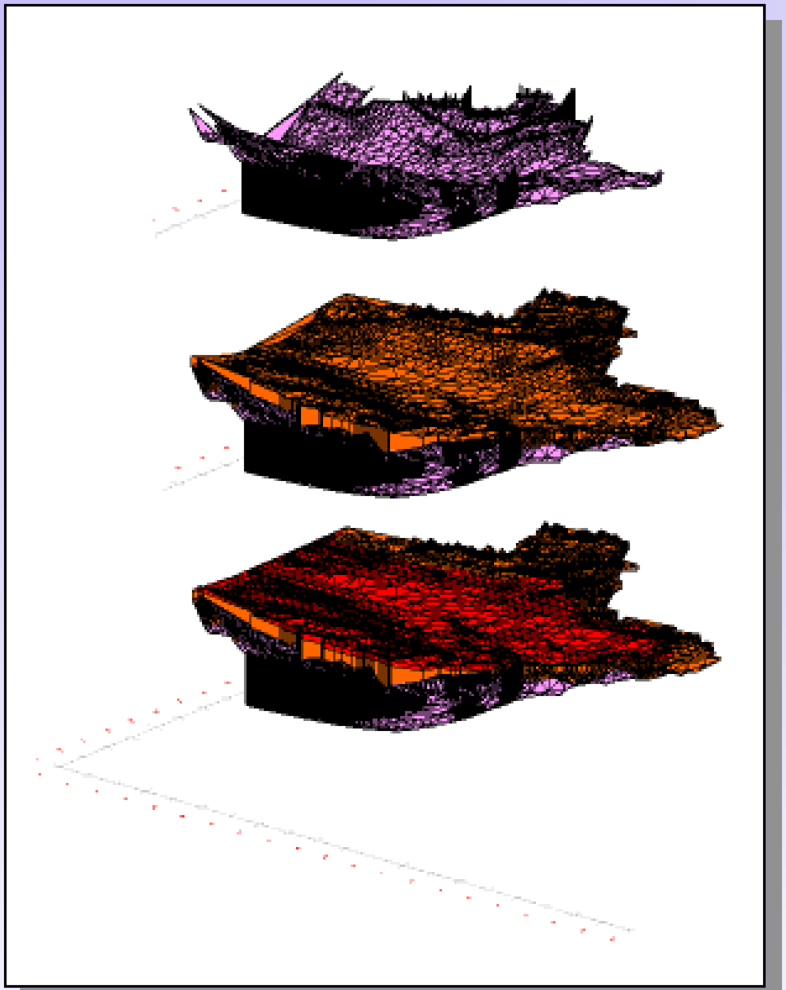
- Combine scalability of multigrid and convergence of conjugate gradient methods
- MG Preconditioning —
  - One standard MG V-cycle in residual CG step, with or without smoothing
  - Ad-hoc semi-coarsening employed for anisotropic grids
  - Operator-induced prolongation and restriction for discontinuous properties
- Scalability demonstrated on 256 node Cray T3D for problems in excess of 50 million unknowns
- Supports rapid simulation

Nested Generation of Stochastic Property Fields Needed for Efficient Monte Carlo Operation



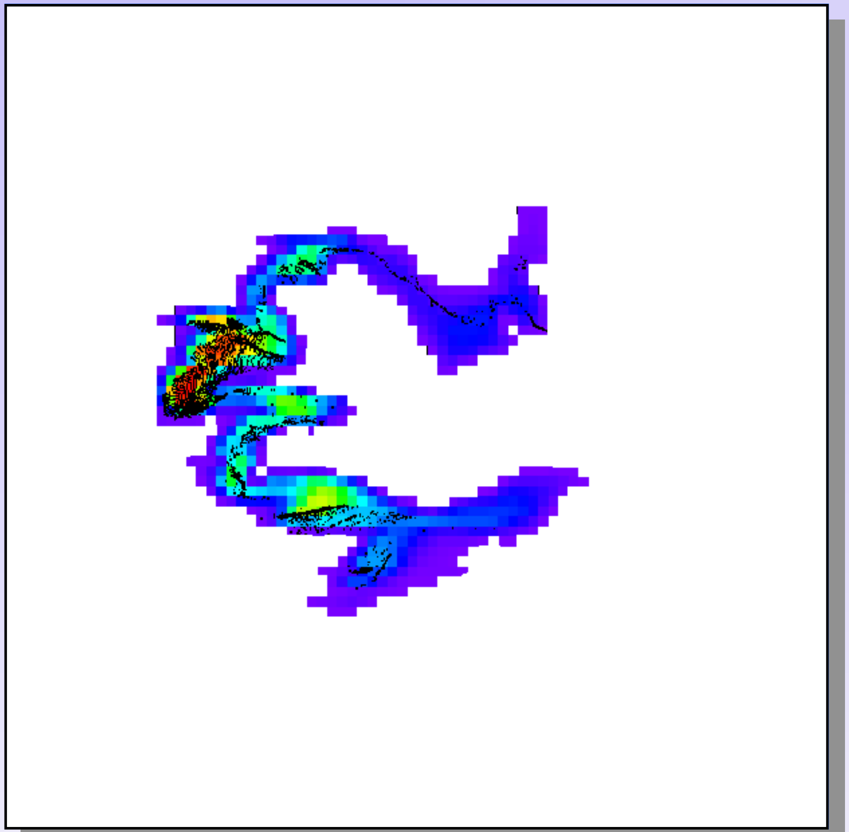
- Nested (parallel) implementation required to eliminate I/O chokepoints
- Current code allows for separate Gaussian Field generation in targeted sub-units of domain
  - Unconditional **Turning Bands Method**, not Scaleable
  - Conditional **Parallel Gaussian Simulator**, Scaleable, but limited in resolution
- Future implementations to incorporate several “indicator simulation” variants based upon the SIS algorithm

Grid-Independent Domain Specification Eases Implementation Across Platforms



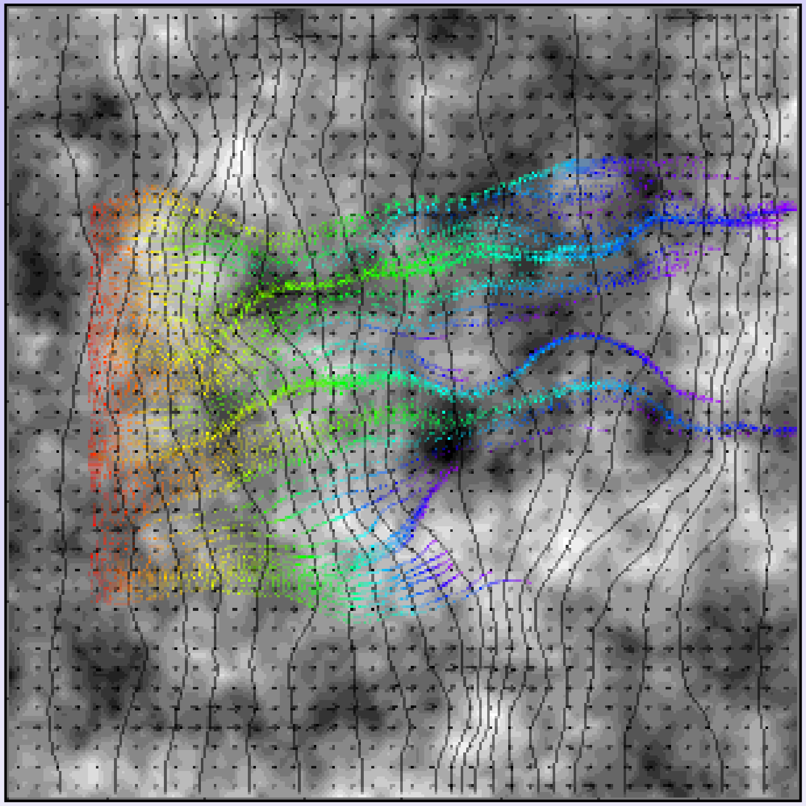
- Reduced data flow lessens I/O chokepoints
- Single specification can be used for coarse or refined applications, across platforms
- Approach —
  - represent HSUs or other subregions as blocks or volumes between triangulated layers
  - assign properties or stochastic model parameters to each subregion
  - conform "block" domain to real boundaries
  - define boundary patches for boundary condition specification
- Based upon GMS (Groundwater Modeling System) interface

Explicit 2nd Order Godunov Advection Algorithm Forms Basis for Transport Module



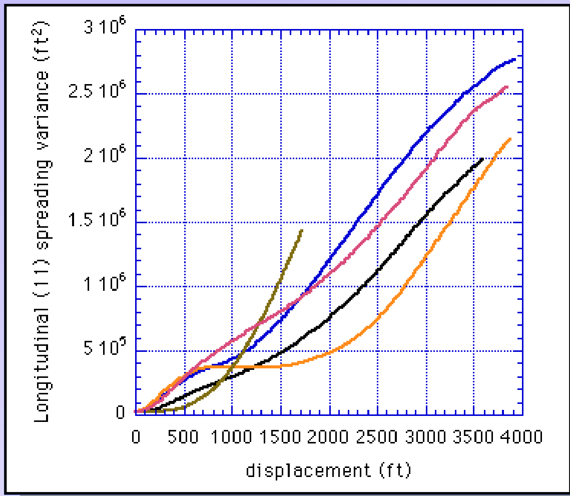
- Explicit approach simple to implement in parallel mode
- CFL condition is overly restrictive in heterogeneous problems
  - allowable time step restricted by global maximum velocity
- "Temporal subcycling" approach expected to ameliorate some of the problem
  - tailor time step in different portions of domains
  - 35 — 75 speed-up factor
- Similar issues in multiphase portion of ParFlow

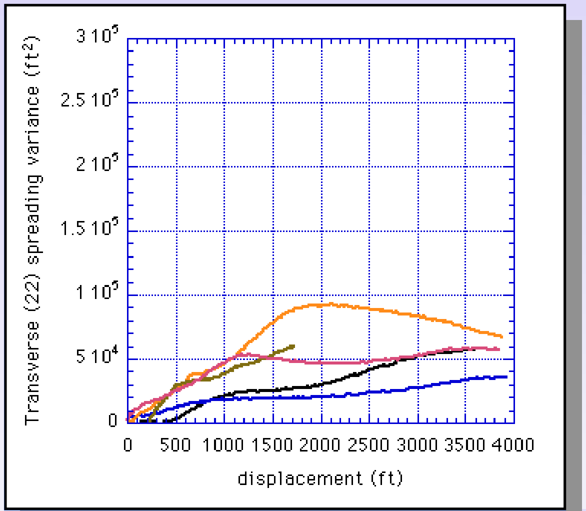
Existing and Future Particle/Streamtube Algorithms Complement 2nd order Godunov Scheme



- Streamtube models shown to be efficient and accurate in many multiphase and density-dependent flow problems
  - attractive for many types of reactive flow and transport processes
  - dispersion and diffusion issues need to be dealt with more carefully
- “External” application easy, internal application needs to be looked at more closely
  - parallel implementation may be easier than some particle algorithms
- Complements existing “external” particle transport models

Applications are the Key to Success with ParFlow

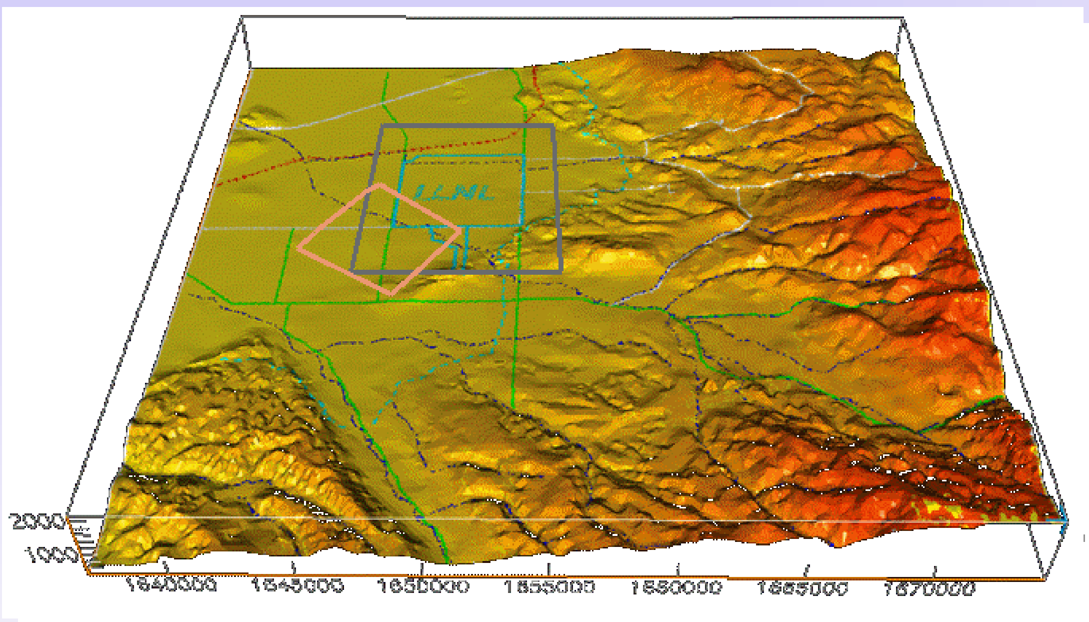




- Traditional uses focus on validation and confirmation of stochastic theories
  - Macrodispersion coefficients, effective hydraulic conductivities, anisotropy, bulk retardation and decay behavior, nonlocal processes, etc.
- Newer applications address a wider spectrum of practical problems
  - Contaminant remediation at LLNL
  - Contaminant remediation at AJAX site in Northern CA
  - Applications to health risk assessment under uncertainty
  - Aquifer management in Orange County, CA
  - Evaluation of hydrologic source term(s) from nuclear testing at the Nevada Test Site

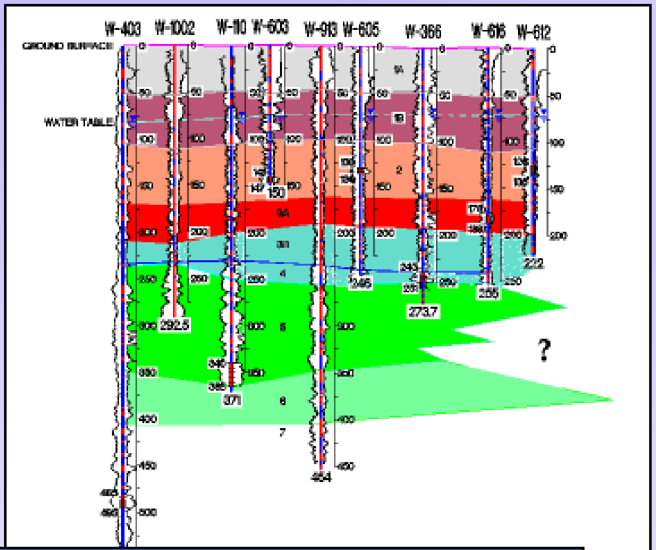
Contaminant Remediation at LLNL

- Superfund Site contaminated with 9 VOCs (TCE and PCE), some tritium, fuel hydrocarbons
- 3D distribution of aqueous solutes in alluvial setting — DNAPL presence not certain

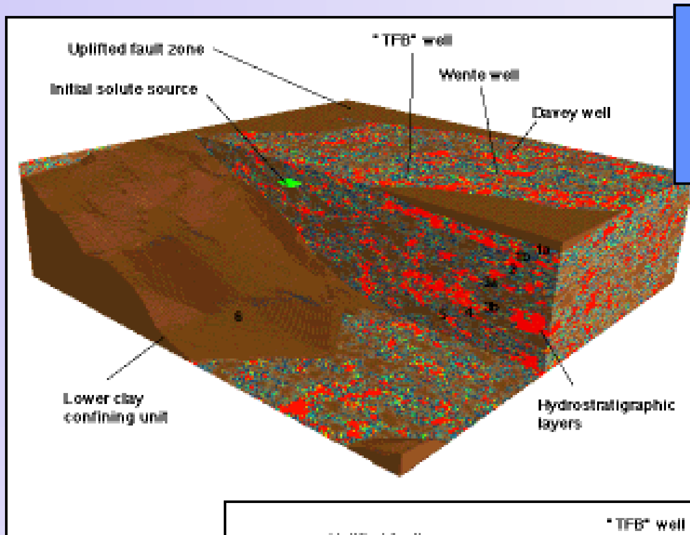


- Regional (2D) simulations are being supplanted with a 3D focus and detailed simulations
- Target — better understanding of
  - historical evolution of contamination
  - interpretation of cross-well interference tests
  - efficiency of pump and treat reclamation
  - uncertainty in recovery predictions

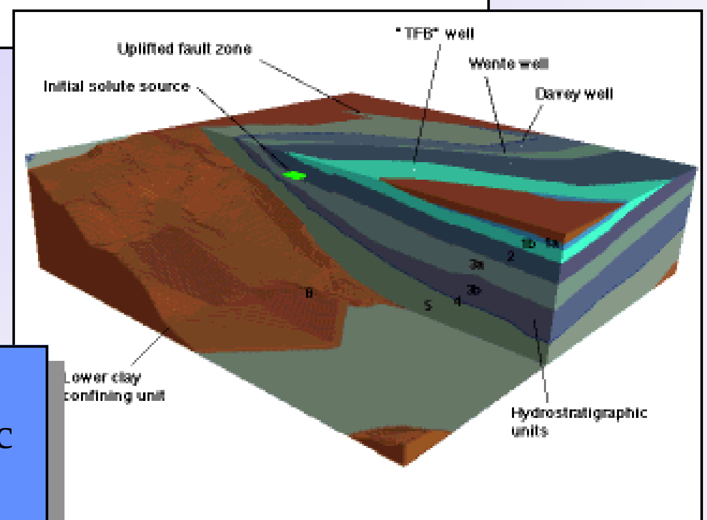
Typical Conceptualization Hierarchy



1. Cross sections, hydraulic, and borehole data

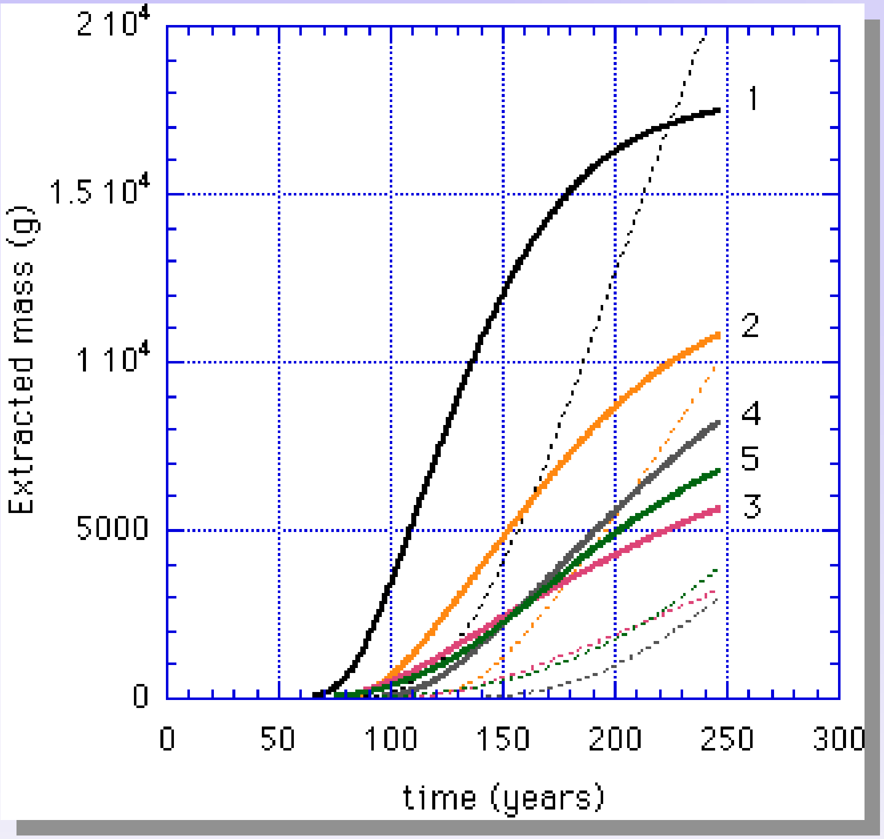


3. Geostatistical realization of internal structure



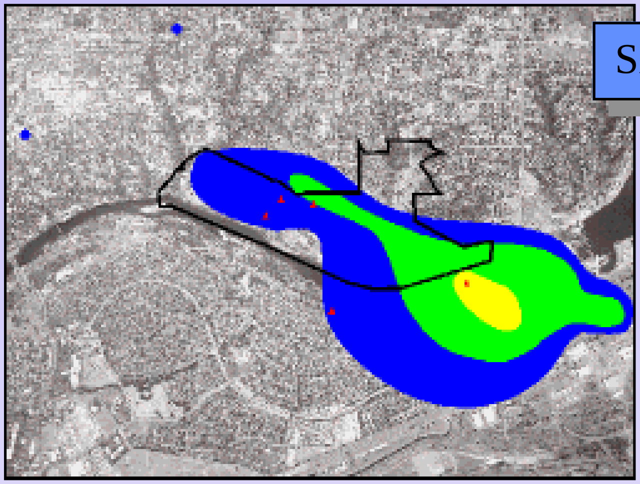
2. Approximate hydrostratigraphic representation

Five Monte Carlo Cycles Illustrate Variability in Source Recovery



- Hypothetical tracer and reactive contaminant source released in LLNL system
- Migration under ambient conditions occurred for 41 yr.
- Migration under one remedial pumping well occurred thereafter
- Variation in recovery illustrates impacts of uncertainty in medium configuration
- Conditioning realizations to available data should lower range of variability

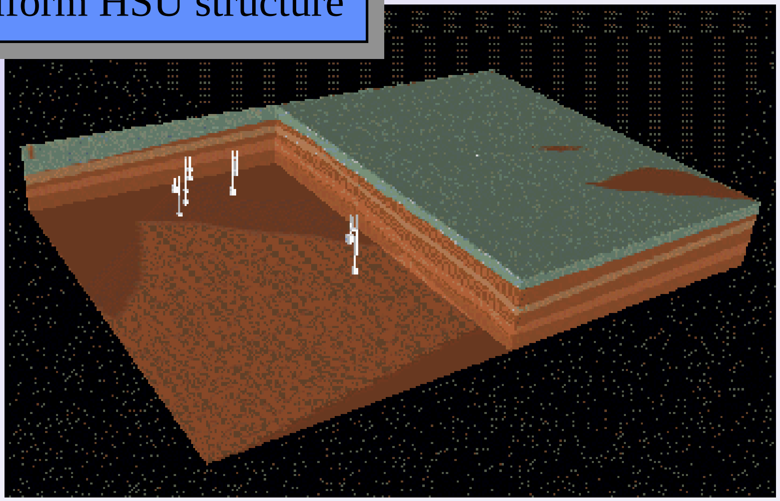
Remediation at AJAX Site in Northern California

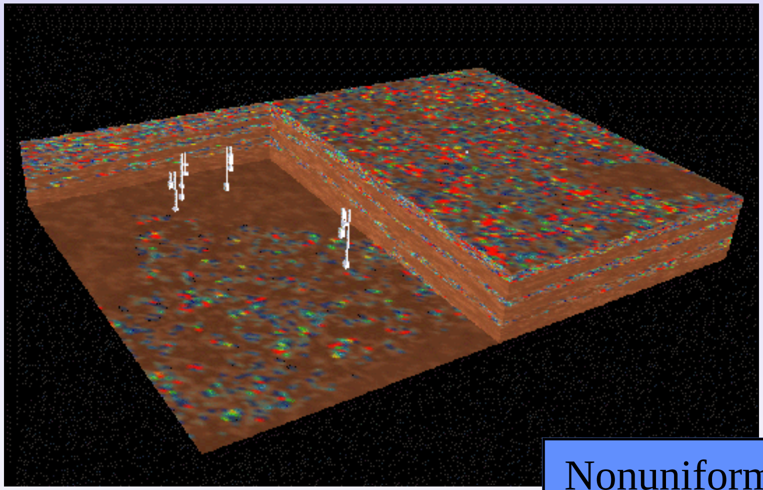


Site

- Site cleanup supervised by industrial partner
- Traditional solvent contamination in a high-profile setting
- Client has blessed ParFlow approach

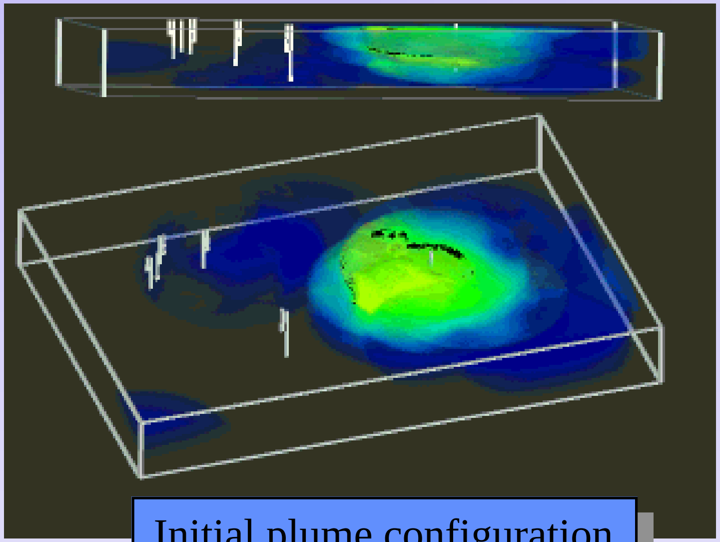
Uniform HSU structure



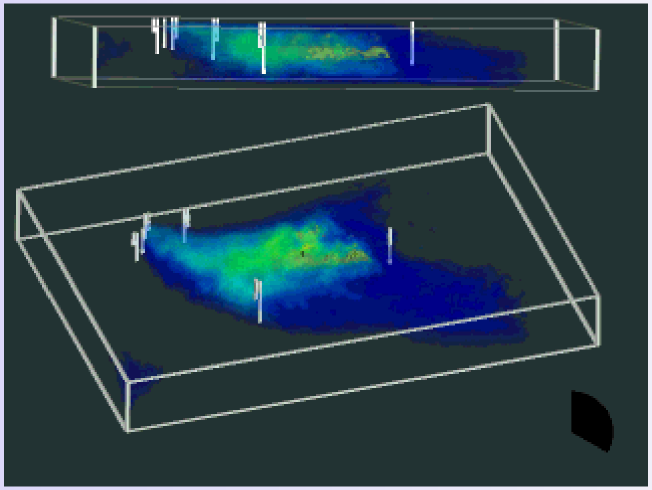


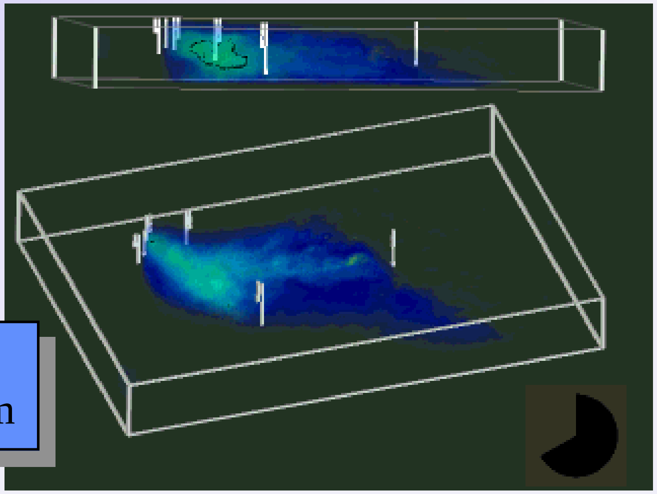
Nonuniform HSU structure

Remediation at AJAX Site in Northern California



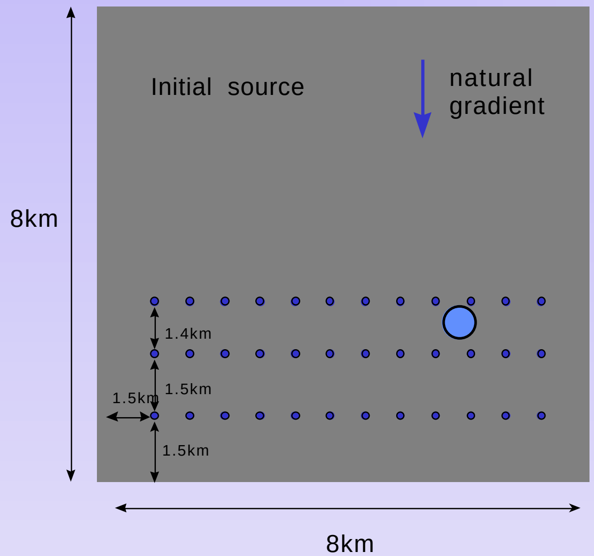
Initial plume configuration



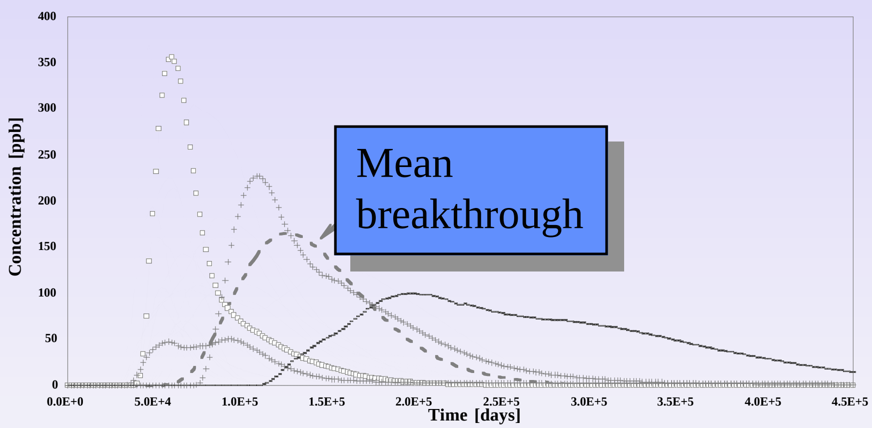


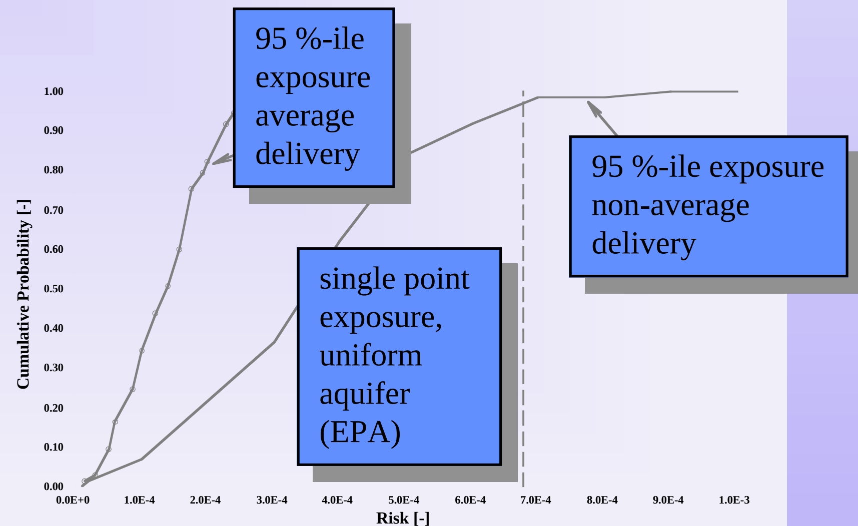
Simulated extraction
on a 1M node problem

Risk Assessment under Uncertainty and Variability

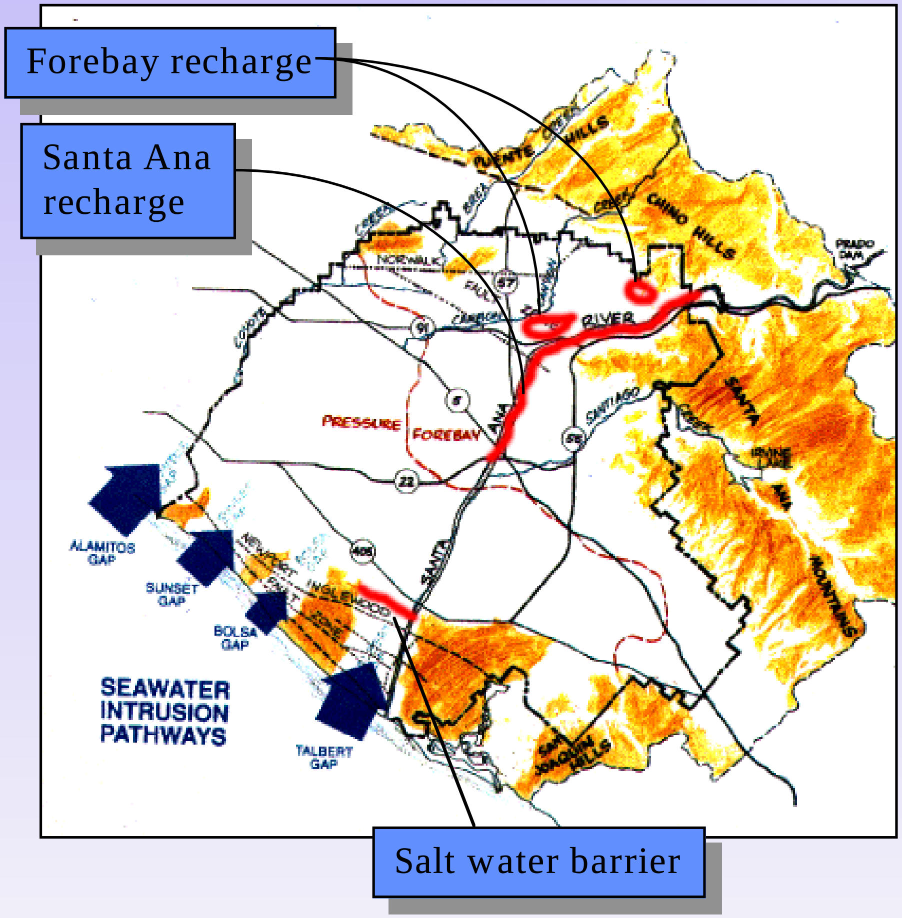


- Exposure and Groundwater Risk assessment under multiple well distribution system
- **Uncertainty** —Monte Carlo analysis of plume evolution in heterogeneous media leads to concentration ensemble at each well
- **Variability** — Evaluate distribution of increased cancer risk over population spectrum



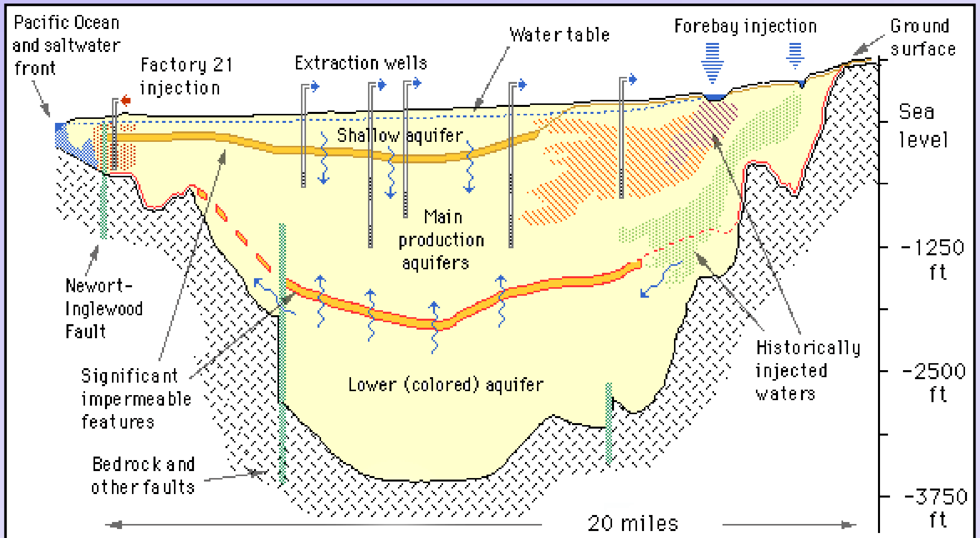


Application of Large-Scale Simulation for Aquifer Management in Orange County, CA

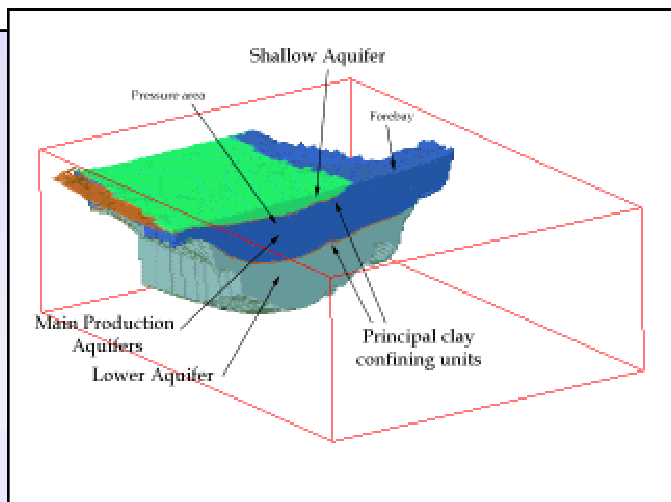


- Groundwater provides 70% of domestic water for over 2 million residents
- Supplemental groundwater provided through recharge of Santa Ana River water and treated wastewaters along river and Forebay recharge basins
- Concerns:
  - who has access to recharged water?
  - what are the residence times of recharged wastewater?
  - how will increased production affect salt water barrier?

OC Aquifer System is Large and Complicated

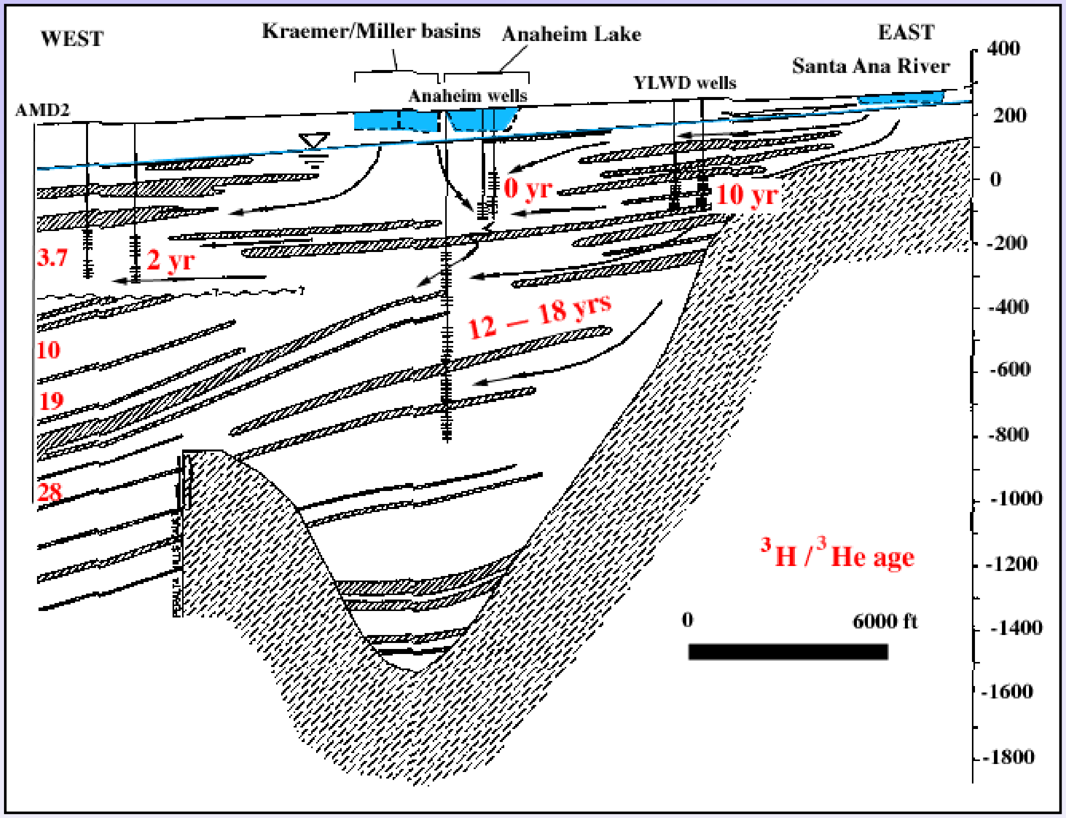


Typical Cross Section



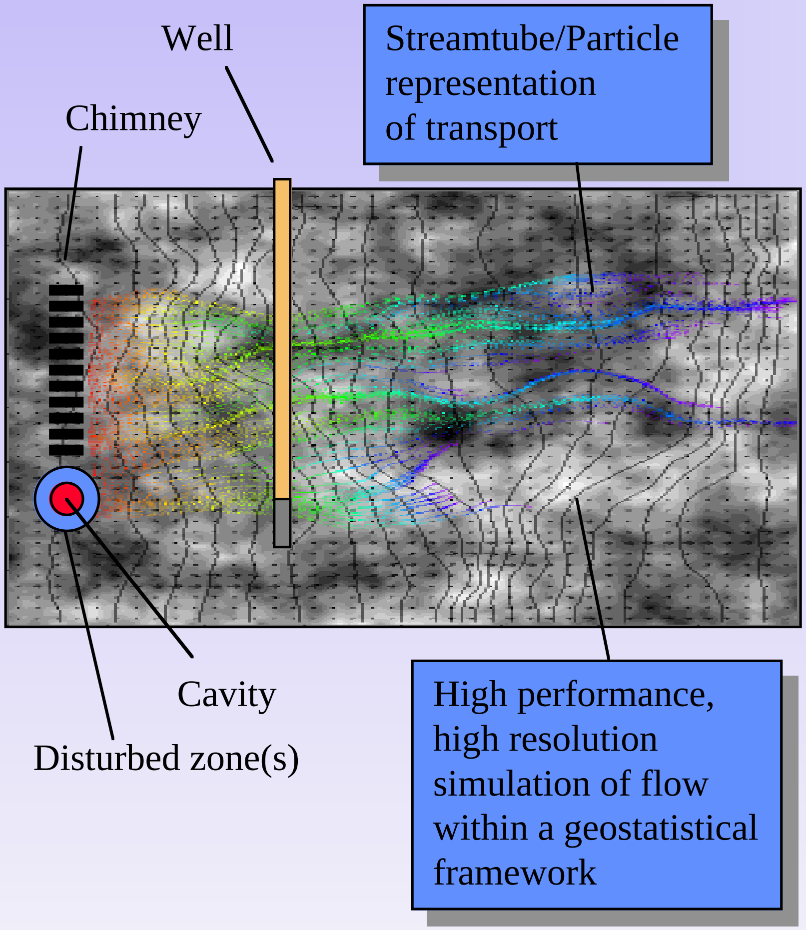
- 20 miles square, three principal units, 4000 ft deep
- 3D resolution important for describing transport pathways and dilution of recharged waters
- Isotopic data suggest travel pathways and water ages
- Geostatistical approach may be required for added interpretation
- Preliminary simulations will begin on a 6.6 million node problem

“High Resolution” Approach



- Generate multiple geologic “realizations” from available borehole, geophysical, and interpretive data
- Reproduce measured data and “character” of finer structure
- Multiple simulations reveal “distributions” of ages at specific points: reproduce interpretations

Evaluation of Hydrologic Source Term from an Underground Nuclear Test at Frenchman Flat, NV



- Focus on the **near field** (~10 R_c) hydrologic regime surrounding a "canonical" saturated zone test in Frenchman Flat
  - Cambric test
  - Reproduce tritium elution curve
  - Address "hypothetical" tests with canonical geologic, hydrologic, or geochemical features
- Develop a detailed, near-field, 3D hydrologic model capable of direct geostatistical flow and transport simulations
- Development / incorporation of simplified geochemical models of sorption/desorption, dissolution, speciation, and colloidal formation and migration for target radionuclides
- Estimate radionuclide fluxes into far-field environment to estimate **risk envelope**

Future

- Improvements in GMS interfaces
- Improved geostatistical representations
- Implementation of streamtubes
- Compressibility effects
- Return to 2 phase problems, Richard’s equation
- Real time I/O of graphics
- Applications, Applications, Applications, Applications, Applications, ...